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EMPulse, a new 3-D simulation code for EMP formation and propagation

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35-word or less abstract:

EMPulse is a new 3-D simulation code for EMP generation and propagation studies. Beginning with the open-source Warp PIC framework, we have added EMP-specific physics models. The code's methods and initial tests are described.

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EMPulse, a new 3-D simulation code for EMP formation and propagation

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EMPulse is a comprehensive and modern 3-D simulation code for electro-magnetic pulse (EMP) formation and propagation studies, being developed at LLNL under a Laboratory Directed R&D (LDRD) initiative that was launched in the fall of 2014. EMPulse builds upon the open-source Warp particle-in-cell code framework which was developed by members of this team and collaborators at other institutions. The goal of this endeavor is a new tool, using methods different from those in common use, and enabling the detailed and self-consistent study of multi-dimensional effects in geometries that have typically been treated only approximately. Here we describe the underlying Warp framework and its capabilities; the models that have been or are being newly developed and incorporated into EMPulse, tests of these models, and number of approaches to increased computational efficiency that we are studying.

I. Background

EMPulse is a comprehensive and modern 3-D simulation code for electro-magnetic pulse (EMP) formation and propagation studies, being developed at LLNL under a Laboratory Directed R&D (LDRD) initiative that was launched in the fall of 2014. EMPulse builds upon the open-source Warp particle-in-cell code framework[1,2,3], which was developed by members of this team and collaborators at other institutions. The goal of this endeavor is a new tool,[4] using methods different from those in common use, and enabling the detailed and self-consistent study of multi-dimensional effects in geometries that have typically been treated only approximately.

Efficient methods for EMP simulation, developed by Longmire and collaborators, are embodied in the CHAP code[5]. CHAP (in its various embodiments, including a modern implementation at LANL[6]) remains a work-horse code for EMP studies in the U.S. The HEMP codes,[7] also heavily used, employ models related to those in CHAP. We have examined a number of assumptions made in CHAP, and in general find them valid for the scenarios targeted by the code's authors[8,9,10]. However, CHAP assumes one-dimensional (spherical) symmetry, with only a limited (and rarely employed) capability for tracking rays that are shifted slightly from the line-of-sight (LOS) in order to include non-spherically symmetric contributions to first order. It cannot accurately treat the full range of problems of interest.

A modern 3-D code has been developed at LANL[11]; it is based on the MCNP package[12] and a high-order FDTD Maxwell solver. The code is useful for scenarios with complex geometry and terrain, *e.g.,* EMP in a city, but in its present incarnation is restricted in the distance over which EMP can be propagated before spurious (numerically induced) dispersion becomes excessive.

The MACSYNC code[13] also employs the MCNP package for generating and tracking Compton electrons, but in contrast with most tools in current use is based upon a Liénard-Wiechert (henceforth, "L-W") formulation, wherein each acceleration of every simulated Compton electron contributes an EMP photon which is tracked to the observer's position. It is readily capable of handling complex geometries, and has offered valuable insights into aspects of EMP physics, for example, effects of the shadowing of some of the gamma rays produced by the burst by optically-thick objects. However, the formulation as it stands imposes considerable difficulty in arriving at the self-consistent time- and space-dependent conductivity needed for accurate attenuation of the EMP as it travels to the observer.

Recently, we have studied aspects of EMP formation and propagation using a new model within EMPulse's Python / Fortran framework known as LWMC (for Liénard-Wiechert Monte-Carlo).[4] Using LWMC, we have benchmarked EMPulse's FDTD Maxwell solver, in particular its numerical dispersion properties, and identified physical mechanisms that had not previously been explicitly called out. For example, the geomagnetic (centripetal) force on a Compton electron is initially normal to the LOS, and even after it has started to gyrate remains principally normal to the LOS. At this time, the drag force also has a component normal to the LOS, oppositely directed to the geomagnetic force. This reduces the amplitude of the generated EMP. A similar effect arises due to scattering events which, on average, cause particles to move more slowly along the pre-scatter direction of their motion. As with drag, the symmetry breaking induced by geomagnetic rotation leads to a net effect on the EMP field.

To benchmark the EMP generation physics in EMPulse, another new model was developed within the Python framework. This model, known as CHAP-lite, includes the classical CHAP approximations such as an "obliquity factor" model for the scattering of Compton electrons and the "high frequency" EM wave approximation. Comparisons of CHAP-lite with CHAP, showing close agreement, are presented in a companion paper.[10] More-complete physics models, including a Maxwell solver that treats backward-going waves properly and detailed models for the collisional scattering of Compton electrons, can be invoked in CHAP-lite for comparisons against FDTD-based EMPulse calculations; these comparisons are briefly described below.

II. Code framework, models, and initial tests

EMPulse builds upon the Warp code base, which offers 2-D and 3-D electrostatic and electromagnetic particle-in-cell (PIC) methods, and has been benchmarked on ion beam experiments, laser acceleration, anti-hydrogen traps, and many other applications.[14] In this framework, the algorithms for physical processes may be thought of as "physics extensions to Python." Input files are Python programs, and the code can be run interactively; it is user-programmable and "steerable" when desired. Computationally-intensive operations are carried out in a Fortran code layer; arrays and scalars from the Fortran are accessible at the Python level, so that users can readily insert diagnostics that run "on the fly" as needed. Users rarely (if ever) must alter the underlying Fortran level.

With EM PIC capabilities in hand, creating EMPulse largely consists of adding EMP-relevant models that were not developed for any prior use of the framework. We have added: a description of the gamma source; Compton electron generation based on the Klein-Nishina model; an atmospheric density model similar to that of CHAP and other codes; models for the drag and scattering of Comptons based on the NBS tables, using improved Monte-Carlo methods (with an exponential integrator); and conductivity models similar to those of CHAP, including both Ohmic and swarm options. The code runs on machines at LLNL's computer center, on local clusters, and on personal computers under Linux or Macintosh OSX.

To date we have benchmarked EMPulse on 1-D example problems with a sub-km thick active-region, comparing the evolution of key quantities against those produced by CHAP-lite, which has itself been benchmarked against CHAP.[9] In Fig 1(a), a 1 kT burst at 30 km altitude with a gamma yield of 0.3% is assumed, and a delta-function pulse of 1.6 MeV gamma photons is assumed to propagate freely to 20 km, and then interact with the air; diagnostic "cuts" are taken every 10 meters. In this case, drag, scattering, and conductivity have been switched off. The vertical coordinate is z, and the horizontal coordinate x. In Fig 1(b), the burst is at 40 km altitude, and the gamma photons are assumed to propagate through vacuum to 30 km; drag, scattering, and Ohmic conductivity were enabled. The modest disagreement in the fields at the greatest depth into the active region is under study; we suspect that the timesteps used in the CHAP-lite run were not sufficiently small for numerical convergence.

III. Future Directions

In addition to benchmarking the new models in EMPulse and overall code operation, we are implementing and exploring a number of routes toward improved performance.

We have begun adaptation of Warp's "Pseudo-Spectral Analytical Time Domain" (PSATD) Maxwell solver to EMP simulation requirements. Because light waves are (effectively) advanced as Fourier modes, the spurious numerical dispersion inherent in FDTD solvers is virtually absent. Pseudo-spectral methods, including "analytical" integration from one timestep to the next, have been known for many years.[15] The recent realization that the finite speed of light enables parallelization of this class of methods has made them suitable for large-scale computations.[16] Because the pseudo-spectral solver in Warp does not incorporate

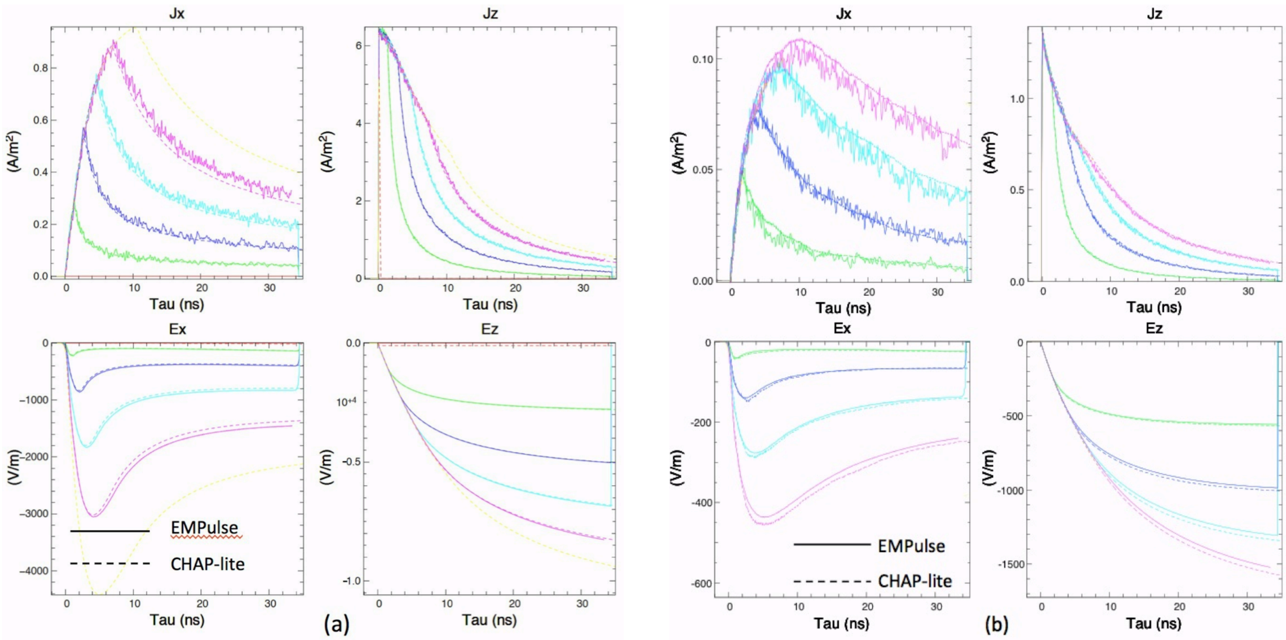

Fig. 1. Comparisons of EMPulse and CHAP-lite; colors denote depths into the active region separated by ten meters (see text): (a) simplified physics; (b) full physics.

terms such as those introduced by a finite conductivity of the medium, we are in the process of generalizing the solver so that it provides this essential capability.

We are also developing a means for terminating simulations of the EMP from a high-altitude burst at a suitable altitude, *e.g.*, 20 km, below which the wave propagates as in free space. At that altitude, outgoing-wave "perfectly matched layer" boundary conditions[17] absorb the EM waves, so they do not spuriously reflect upward into the simulation domain. The field values on grid nodes just above the PML contain the information needed for computation of the EMP waveform as seen by ground observers.

The initial rise of the EMP at the observer's position is governed by processes close to the LOS. Resolving the rise sets the required spatial and temporal resolution near the LOS. Mesh refinement (MR) may allow us to use increasingly coarse zoning away from the LOS. Also, resolution of structures, obscuring objects, and terrain may be more efficiently accomplished. The EM MR capability from Warp[2] is available within EMPulse; its use for EMP studies remains to be explored.

Operation in a Lorentz-boosted frame of reference has revolutionized PIC simulations of laser-based acceleration and of "electron cloud" buildup in particle accelerators.[18,19] In those applications, use of an optimal frame in Warp allows disparate space and/or time scales to be brought closer together ("Lorentz contraction"). Because events that are simultaneous in the lab frame are not simultaneous in the boosted frame, the approach is nontrivial; for example, "snapshot" diagnostics in the lab frame must be generated from a series of data dumps in the boosted frame. We plan to explore the utility of this approach for EMP.

Finally, we are considering a "hybrid" approach that would combine the grid-based EMPulse field solution with either a Jefimenko[20,21] or a L-W model, which would "ride atop" the main code. Since these approaches are "dispersionless," either would offer an alternative prediction of the field at any desired position, as a cross-check of the FDTD field solution's accuracy.

Because supercomputing resources are available, none of these methods is essential to the operation of EMPulse; still, it is our hope that a combination of them will make routine usage convenient.

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